COMPUTATIONAL FLUID DYNAMICS TECHNOLOGY FOR HYPERSONIC APPLICATIONS

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Abstract

Several current challenges in computational fluid dynamics and aerothermodynamics for hypersonic vehicle applications are discussed. Example simulations are presented from code validation and code benchmarking efforts to illustrate capabilities and limitations. Opportunities to advance the state-of-art in algorithms, grid generation and adaptation, and code validation are identified. Highlights of diverse efforts to address these challenges are then discussed. One such effort to re-engineer and synthesize the existing analysis capability in LAURA, VULCAN, and FUN3D will provide context for these discussions. The critical (and evolving) role of agile software engineering practice in the capability enhancement process is also noted.

Introduction

Computational fluid dynamics (CFD) is the numerical simulation of flowfields through the approximate solution of the governing partial differential equations for mass, momentum, and energy conservation coupled with the appropriate relations for thermodynamic and transport properties. Aerothermodynamics is the branch of fluid dynamics that focuses on the effects of thermodynamic and transport models on aerodynamics and heating. It is especially focused on conditions of hypersonic velocities where the energy content and exchange between kinetic, internal, and chemical modes in the flow precludes the otherwise common use of calorically perfect gas assumptions. Computational aerothermodynamics is therefore defined in exactly the same manner as CFD, with the added emphasis that high temperature gas effects on pressure, skin friction, and heat transfer are included in the numerical simulation. The fundamental role of computational aerothermodynamics is the simulation of aerodynamic forces and heating for external and internal high speed flows. Reference 1 presents a review of recent applications for access to space and planetary missions.

The approximate solution of the governing equations requires that the domain be subdivided into many small control volumes. The accuracy of the solution depends upon a variety of factors; the most critical factors are the size of each control volume, the orientation of its boundaries relative to a variety of flow features, and the order of accuracy of the discretization. At the risk of belaboring the obvious, note that hypersonic flows routinely involve extremes of pressure, density, and temperature separated by shocks, expansions, shear layers, and boundary layers. These extremes in conditions and topology of flow structure complicate computational aerothermodynamic simulation. The ability to orient a grid with evolving flow structures is particularly challenging. For example, accurate simulation of heat transfer requires adequate resolution of the boundary layer (or merged layer) and accurate representation of conditions at the boundary-layer edge. Conditions at the boundary-layer edge in turn, particularly in the stagnation region of hypersonic flows, are dependent on entropy carried along streamlines from the shock. Any irregularities in the captured shock create associated irregularities in entropy that feed the rest of the domain. Further complicating the simulation is the fact that the natural stability properties of upwind schemes so often used in hypersonic applications are in turn most poorly realized in the broad, stagnation region of blunt bodies where system eigenvalues are small.

Nevertheless, computational aerothermodynamic tools that generally do a good job in handling the difficulties of steady, laminar, hypersonic, blunt body and attached flow simulation have evolved over the past 15 years. The greatest uncertainty in such applications is the validation of physical models for a host of non-equilibrium processes[2]. Greater challenges are encountered in the

simulation of separated flows, complex shock-shock and shock – boundary-layer interactions, prediction of transition, time-dependent flows, and plasma flows. The application of unstructured grid methods for such three-dimensional simulations (even the relatively simple blunt body problem) has proven to be especially challenging when heat transfer is required as will be discussed herein.

The goal of this paper is to reflect on the needs of computational aerothermodynamics in order to meet these challenges. Some of the approaches discussed here are under development within the High Energy Flow Solver Synthesis[3] (HEFSS) project at NASA Langley Research Center. This project combines the physical models and simulation capabilities in the structured codes LAURA[4] (focus on external, hypersonic flow simulations) and VULCAN[5] (focus on internal, scramjet flow simulations) into the unstructured flow solver FUN3D[6] (perfect gas flow simulations with adjoint-based design and optimization capabilities). The ultimate goal of this project is to develop robust schemes with quantified uncertainties requiring minimal user intervention. In this endeavor to re-factor existing sources we modularize the code to simplify future coupling with other physics.

Grid Requirements

Criteria: The HEFSS team is investing in unstructured grid technology, including the use of mixed elements - tetrahedron (tets), prisms, pyramids, and hexahedron (hexes) - as the underlying support for future hypersonic flow simulation. We defer any investment in patched or overset multiblock structured grid systems at this time. The rationale for this approach is based on our assessment of current and anticipated future capabilities for grid generation and grid adaptation. This assessment considers: (1) efficiency in the initial generation of a "reasonable" grid over complex configurations; (2) ability to adapt the grid to flow structures (steady and time-dependent) and changes in parameterized structures on the vehicles; and (3) solution quality and efficiency on a "good" grid using best available algorithms. A "reasonable" grid is one that will accommodate a converged solution with at least approximate resolution of flow structures. It provides an initial condition for future adaptation and refinement. A "good" grid is one that will produce a grid converged solution such that an additional refinement will result in dependent variable changes within user specified tolerances.

Initial Generation: Unstructured grid generation on complex configurations is already judged superior to structured grid capabilities for initial grid generation. As an example, consider the grid shown in Fig. 1 and Fig. 2 which is discussed in Reference 7. A grid around mated ascent vehicles, including a fine grid near all solid surfaces to resolve boundary layers, was generated in approximately four hours (including all user interactions) from a clean CAD file. A subjective judgment of the time required to create an equivalent, multiblock structured grid using continuous or patched interfaces is on the order of days to weeks. The time to generate an overset, structured grid is estimated to be approximately one day. The extra time in these cases derives from the topological decisions required by the user so that the grid will be sufficiently adaptable to accommodate solution quality.

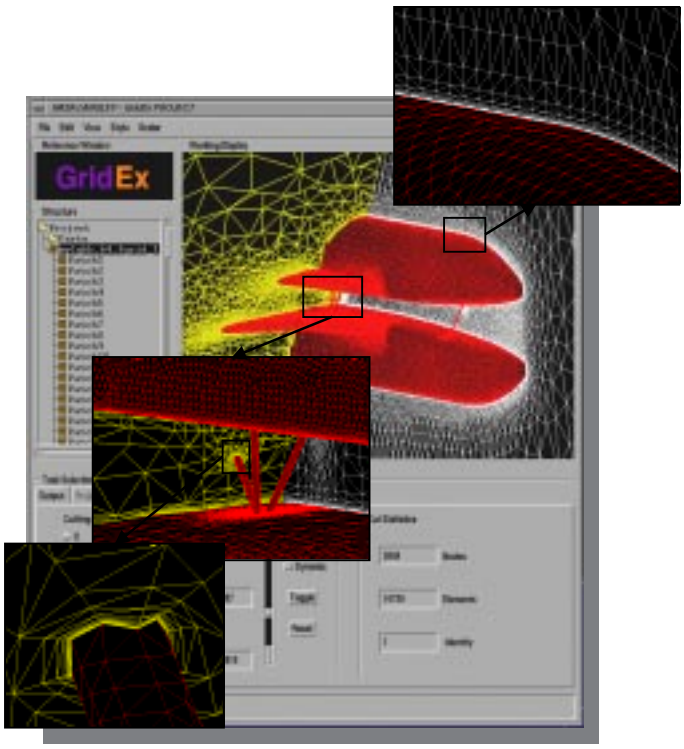

Fig. 1: GridEx application of unstructured grid for simulation of viscous, hypersonic flow over mated reusable launch vehicle system.

Ability to Adapt: The ability to adapt structured grids versus unstructured grids for hypersonic applications is considered to be a draw at present, with unstructured capability advancing rapidly. The external hypersonic flow, structured grid solver LAURA[4], for example, routinely applies quasi-one-dimensional adaptation as part of the solution procedure to align a structured grid with the captured bow shock and control near-wall grid size and grid stretching factors to obtain grid-converged heating rates. However, a lot of time goes into the

grid generation process in order to enable such adaptive capability for complex configurations, and some topologies (e.g. elevon gaps as seen in inset of Fig. 2) are not amenable to such simple adaptation strategies. Many other solution-adaptive tools are available to adjust grid spacing based on user specified, weighted functions of gradients (feature based adaptation) but defining the weight functions is often more art than science in order that all flow structures are adequately resolved.

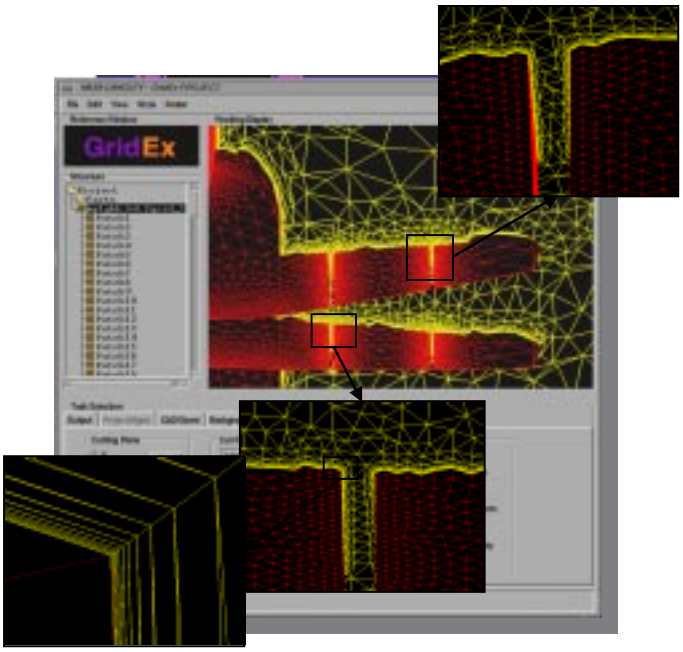

Fig. 2: Details of unstructured grid in elevon gap for RLV application. Scalloped edges are artifacts of presentation of tetrahedral facets.

Feature based adaptation is routinely applied to unstructured grids as well. But unstructured grids provide additional degrees of freedom that enable local enrichment, coarsening, and re-orientation (edge-swapping) without propagating these effects throughout the domain. However, strategies for anisotropic adaptation are required across shocks and shear layers to prevent excessive numbers of nodes from being drawn into the high gradient regions. As an example, the method of Ref. 8 has been applied to Mach 3 flow (inviscid) through a scramjet inlet and Mach 2 flow (viscous, Re 10000) over a NACA 0012 airfoil showing very crisp looking captured shocks across tightly clustered, high aspect ratio triangles (two-dimensional test cases). The algorithm examines the eigenvalues and eigenvectors associated with the Hessian of each dependent variable and derives a transformation based on this geometric information that guides directional refinement. It also enforces a surface boundary orthogonality condition to improve solution quality of skin friction. This issue is likely important for the simulation of heating in hypersonic applications as well.

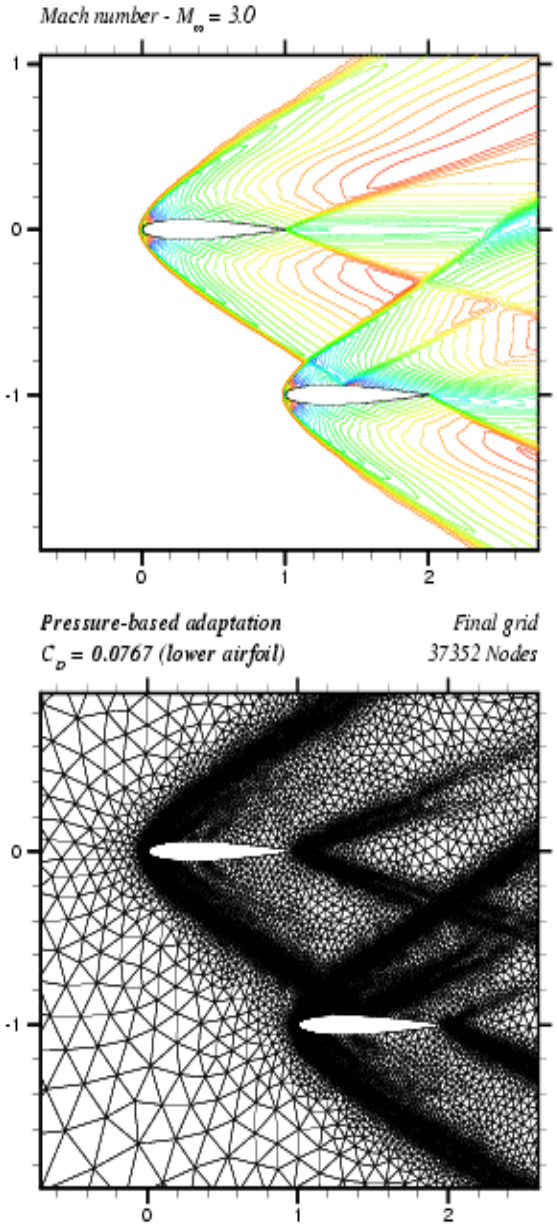

Fig. 3: Mach number contours and feature-based, isotropic adapted grid from Venditti[9] for Mach 3, inviscid flow over airfoils.

Adjoint-based grid adaptation is a recent development that refines mesh as a function of user defined error tolerances. The adjoint equations arise from the linearization of the effects of residual changes at every node on an output function (lift, drag, heating). A user can specify the desired

tolerance on the output function and the adaptation process continues until the tolerance is met or system resource limits are exceeded. In this sense, adjoint adaptation is an objective error minimization technique whereas feature adaptation is a subjective error reduction technique.

An example of adjoint-based adaptation and feature-based adaptation applied to supersonic flow over a pair of airfoils is shown in Fig. 3 and Fig. 4 taken from Ref. 9 and 10. The objective function in this example is the drag on the lower airfoil. The adjoint adaptation yields the same drag coefficient as the Hessian based adaptation to about 0.013% using nearly a factor of ten fewer nodes. Note that anisotropic adaptation has not been included in this example but the capability is currently being tested within HEFSS.

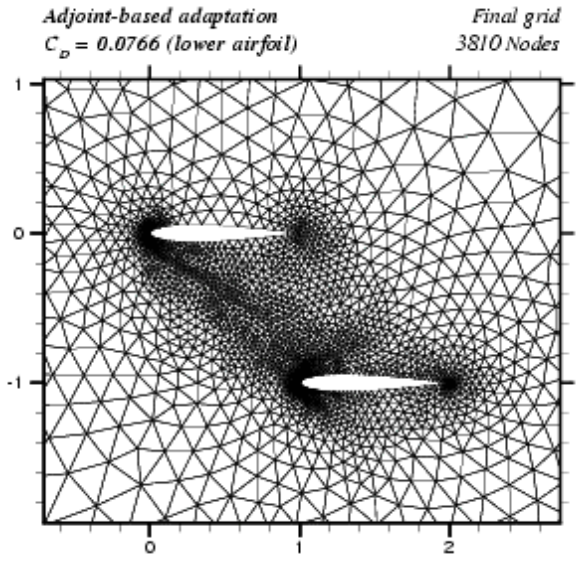

Fig. 4: Isotropic, adjoint-based grid adaptation to obtain grid converged drag on lower airfoil from Venditti[9]. Only parts of flow required to get grid converged drag on lower airfoil are resolved.

It is worth noting that the adjoint equation set provides capability for configuration design and optimization[11]. This capability is currently applied to perfect-gas, low speed to transonic applications in HEFSS. It has not been applied to hypersonic applications because of uncertainty in the choice of optimum algorithm (reconstruction, limiting) required for flow simulations including strong shocks. Still, it is anticipated that this capability will be of fundamental value and was one of the major reasons for choosing the FUN3D code as the baseline for extensions to the hypersonic domain.

Solution quality and efficiency:

Structured grid solvers are currently superior to unstructured grid solvers as regards quality and efficiency for viscous, hypersonic flow applications including heat transfer. This assertion, based on personal observations, ignores the time required to generate an initial grid and assumes that the number of nodes in both approaches is comparable. Unstructured grid solvers carry an overhead associated with connectivity of nodes, edges, and volumes – particularly in the case of mixed elements. The convergence rate of unstructured solvers, especially in the presence of strong shocks is slower than structured grid algorithms. This behavior is thought to be a consequence of greater problems with "ringing" associated with the application of limiters in the flux reconstruction algorithms and with less efficient implicit relaxation algorithms but more research is required to confirm such speculation.

The solution quality concern stems from observations of blunt body stagnation region heating in 3D using HEFSS on simple test problems involving cylinders and spheres. (This issue will be discussed in more detail in the Algorithms section.) Heating contours in these tests display fair to poor symmetry in the stagnation region, depending on the reconstruction algorithm, whereas symmetries are very good away from the stagnation point. It is believed that unstructured-grid-induced irregularities in the captured shock promote entropy gradients that feed directly to the boundary layer edge in the stagnation region. These irregularities tend to be dissipated downstream as the entropy layer enters the boundary layer. The tested grid in the cylinder case was entirely composed of tets derived from an adapted, structured grid. The diagonals inserted into the structured grid to create the tets were all oriented identically; creating a highly biased grid that provides an extreme test case. (A literature search for similar tests focused on 3D heating was unsuccessful.)

Caveats:

(1) The problem of relative motion of two rigid bodies where boundary layer resolution is required on each body is probably better suited to overset grid algorithms. Both structured[12] and unstructured[13] grids may be used as the baseline discretization.

(2) The "unstructured" Cartesian grid method CART3D[14] is a highly efficient alternative to traditional unstructured grid approaches in terms of time to generate and refine a grid and in terms of time to generate a solution on the grid. This approach employs a structured, rectangular grid system throughout the domain (Fig. 5) but enables local refinements to better resolve regions of high curvature in the body and high gradient in the flow.

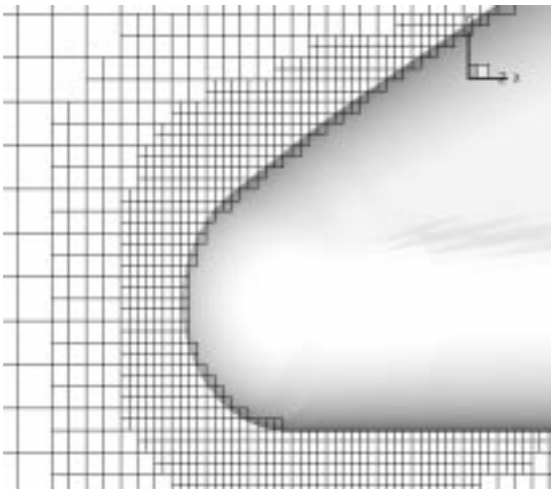

Fig. 5: CART3D grid over nose of X-34.

Preliminary tests of the code for inviscid, hypersonic applications indicate it is very attractive for initial rapid screening of inviscid aerodynamics and can be used to drive boundary-layer codes to obtain convective heating using the axisymmetric analog, notwithstanding some concerns associated with effects of stair-stepping cuts across curved surfaces and shocks. The inviscid plus boundary layer analysis (structured or unstructured) is still the most efficient method for defining heating levels over large acreage areas of attached flows over hypersonic entry vehicles.

(3) The perspective throughout this presentation is on Reynolds-Averaged Navier-Stokes equations which require fine resolution in only one direction (anisotropic adaptation to high aspect-ratio cells) to resolve boundary-layers, shear layers, and shocks (see caveat (4)). External hypersonic flows generally feature broad, thin shock layers that also are most efficiently resolved with high aspect ratio cells (though not as high as required for the boundary-layer). Future applications using Large-Eddy Simulations[15] (LES) require a more isotropic resolution of sub-boundary-layer scale fluctuations across the boundary layer for turbulent flow solutions. This path is not being pursued now in HEFSS because availability of resources for even modestly complex configurations is too far (~15 years) in the future[16]. However, LES for hypersonic applications should be investigated on unit, benchmark problems to prepare for that future.

(4) It is not clear if hexagonal or prismatic elements with faces parallel and orthogonal to shocks are preferred for shock capturing in the context of an otherwise unstructured system. Structured-grid algorithm experience with LAURA shows that fine grid resolution across the shock is not as important as alignment with the shock. Skewed faces across a captured shock may introduce kinks with effects that are evident downstream. Anisotropic adaptation as cited earlier in Ref. 8 appears be an easier approach to the challenge at the expense of additional grid resources. More focused research on 3D hypersonic, blunt body flows with attention to heat transfer is required to resolve this issue.

Algorithm Concerns

Reconstruction and Limiters: Reconstruction refers to the algorithm used to derive the right and left states across a cell wall required in the flux definition in finite-volume, approximate Riemann solvers. Limiters refer to the algorithm used to constrain the reconstructed right and left states to prevent introduction of new extrema in the flowfield. Engagement of a limiter typically reduces the local order of accuracy of the reconstructed flux from 2nd to 1st order. The effects of various linear reconstruction techniques on unstructured meshes are discussed in Ref. 17 by Aftosmis et al. They note an increased degradation of solution quality associated with engagement of limiters on triangular (unstructured) meshes as compared to quadrilateral (structured) meshes. They also note that the use of directional limiting (local engagement of the limiter for each edge direction) as opposed to a global limiting (engagement of the limiter considering all directions emanating from a node) produced higher quality solutions. These observations are consistent with behavior observed in the HEFSS benchmark simulations, to be discussed subsequently.

A high level overview of flux definition in HEFSS is provided below though several important details (eigenvalue limiting, flux reconstruction variable set, eigenvector scaling) are omitted. The detail here is sufficient to provide context for the sensitivity of stagnation heating as a function of the reconstruction algorithm. The basic algorithm uses the divergence theorem (Green-Gauss) for viscous gradients and Roe's method[18] for inviscid flux:

$$f = \frac{1}{2}\left[f_L + f_R - R^{-1}\left|\Lambda\right|\left(d\tilde{q} - d\tilde{q}_{lim}\right)\right] \quad (1)$$

where

$$d\tilde{q} = R\left(q_L - q_R\right)$$

R and R^{-1} are the row and column eigenvector matrices of the flux Jacobian and Λ is the corresponding diagonal matrix of eigenvalues. Two options are offered here to reconstruct the left (L) and

right (R) states. The first (Option 1) uses a least squares gradient[19] with a limiter function by Barth[20] or Venkatakrishnan[21]. The term $d\tilde{q}_{lim}$ in Eq. 1 is identically zero for Option 1. The second (Option 2) uses the nodal values for the left and right states. Option 2 achieves second-order spatial accuracy with the Symmetric Total Variation Diminishing[22] (STVD) scheme applied as a directional limiter (function of edge orientation) as follows:

$$d\tilde{q}_{lim} = 2\ \text{minmod}(d\tilde{q}_L, d\tilde{q}_R, d\tilde{q}, \frac{1}{4}(d\tilde{q}_L + d\tilde{q}_R))$$

$$d\tilde{q}_M = R[d\vec{s} \cdot \vec{\nabla} q_M]$$

$$d\vec{s} = [(x_L - x_R)\vec{i} + (y_L - y_R)\vec{j} + (z_L - z_R)\vec{k}]$$

The gradients $\vec{\nabla} q_M$ at nodes (M = L or R) are computed using the identical, unlimited least squares formulation from Option 1. The STVD limiting in Option 2 and the Venkatakrishnan limiting in Option 1 are observed to diminish but not eliminate overshoots and undershoots in temperature and pressure in the vicinity of strong shocks. A pressure ratio weighting function is used to smoothly switch to first-order in the vicinity of strong shocks to augment the limiting process in Option 2. Options 1 and 2 use identical formulation of the viscous terms.

Fig. 6: Structured grid and equivalent uniformly biased unstructured grid in symmetry plane over cylinder for hypersonic test case.

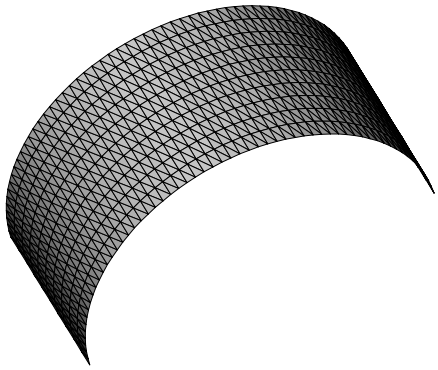

Fig. 7: Uniformly biased, unstructured surface grid derived from structured grid with ten spanwise cells.

Benchmark Tests: Benchmark cases for hypersonic flow over a sphere and a cylinder at V_∞ = 5000 m/s, ρ_∞ = 0.001 kg/m^3, T_∞ = 200 K (approximately Mach 17) consistent with earlier LAURA benchmarks, have been intensively worked during the HEFSS code development process. Cases presented here are for single species N_2 but thermochemical equilibrium and nonequilibrium options are operational. The structured LAURA grid, adapted to align with the bow shock, is shown in the bottom part of Fig. 6. The unstructured grid for the HEFSS tests (top of Fig. 6) is formed directly from the structured grid. Both grids are three-dimensional (structured hexahedra (hexes), unstructured tetrahedral (tets)). The unstructured surface grid is shown in Fig. 7. The grid is highly biased with diagonals running in the same direction. The biasing is intentionally retained to test simulation quality under adverse conditions. Spanwise symmetry of the solution across the bias is easily monitored. Comparisons to the structured grid LAURA results are also available in the evaluation process.

The single spanwise cell simulation results with Option 2 (STVD) are shown in Fig. 8. In this case there are no interior nodes in the spanwise direction. The HEFSS results for heating and pressure at surface nodes (indicated by symbol location) on the front and back plane are presented; the pressure symbols on the front and back plane exactly match, the heating levels exhibit a very small offset (less than half a symbol height). Good agreement with the LAURA reference is achieved and the near perfect over plotting of the front and back plane results indicates excellent spanwise constancy.

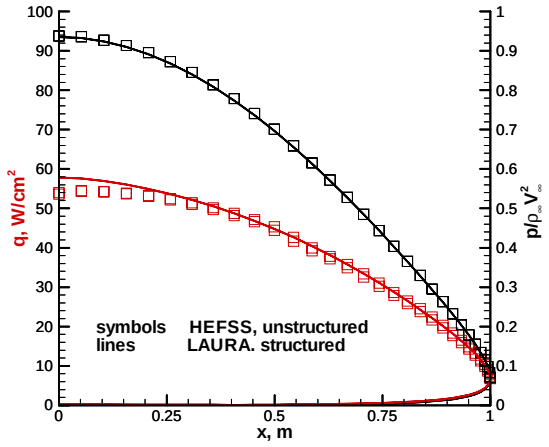

Fig. 8: Pressure and heating distribution for cylinder test case with 3D, uniformly biased, unstructured grid across one spanwise cell. Front and back symmetry planes results essentially overplot as expected for perfect spanwise uniformity.

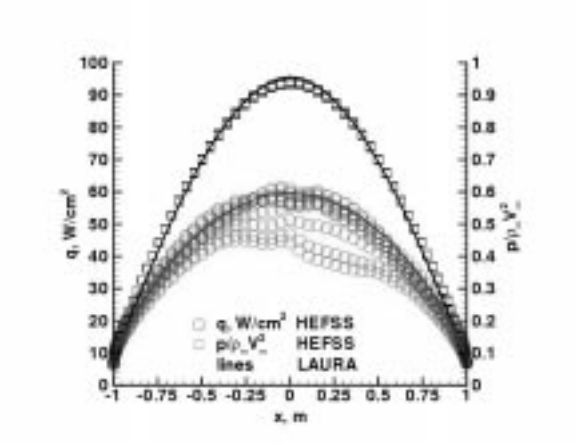

Fig. 9: Pressure and heating distribution for cylinder test case with 3D, uniformly biased, unstructured grid across ten spanwise cells with Option 2. Every surface node is plotted.

The ten spanwise cell simulation results with Option 2 (STVD) are shown in Fig. 9. In this case there are nine interior nodes on each spanwise line as shown in Fig. 7. The value at every surface node from the HEFSS simulation is plotted. The eleven spanwise nodes for pressure again show excellent constancy but the heating shows significant spanwise variation approaching the y=0 plane (Fig. 10), with maximum spread in the stagnation region and solution quality improving away from the stagnation region. The average value of both the pressure and heating continue to be in good agreement with the LAURA results. The equivalent result using Option 1 with the Venkatakrishnan limiter is shown in Fig. 11.

In this case, pressure constancy is slightly degraded and more significant asymmetry in heat transfer is evident. Though not shown, the Option 1 results with the Barth limiter are of poorer quality and appear more like a first-order result. In all cases, the symmetry of shock layer contour plots of pressure, temperature, and Mach number show consistent trends; the spanwise symmetry properties of the Option 2 path are superior to all other tested options.

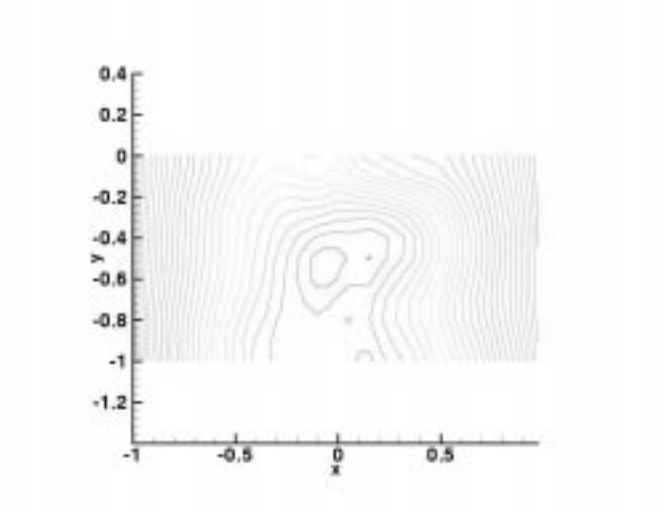

Fig. 10: Surface heating contours on cylinder from Option 2.

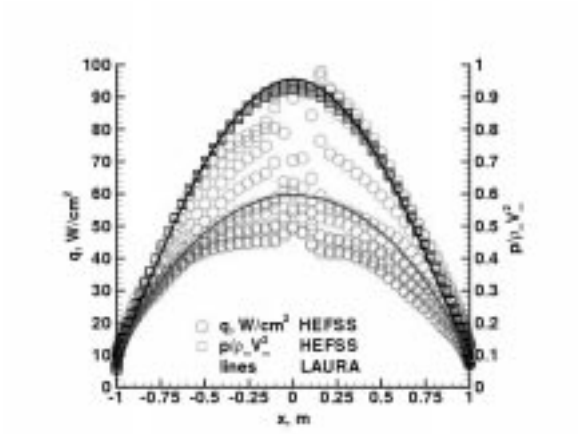

Fig. 11: Same as Fig. 9 with Option 1 and Venkatakrishnan limiter.

These results demonstrate that solution quality for stagnation point heating behind strong shocks using tets all the way to the wall is poor using any of the reconstruction options discussed herein. Improvement is expected if prisms are applied in the near wall region but this option was not available in time to be discussed here within HEFSS. It is unfair to lay all of the blame on the Green-Gauss formulation of viscous gradients across high aspect ratio cells when the results are so obviously sensitive to the

higher order inviscid formulation. In any case, the freedom to utilize tets across the entire domain – even to the wall – provides the greatest flexibility for future grid adaptation. Note that the first-order, edge-based reconstruction in Eq. 1 only involves information at nodes R and L. A conjecture is offered that a truly multi-dimensional reconstruction of the flux at every face could overcome some of the simulation quality issues noted above. A multi-dimensional upwind (MDU) algorithm for high speed flows has recently been developed[23,24]; it is not yet known how it would perform on the ten-spanwise-cell cylinder test problem for hypersonic, blunt-body heating.

Shock capturing: Special algorithms for shock capturing are obviated if anisotropic adaptation and/or a multi-dimensional reconstruction algorithm provide acceptable solution quality. If locally orthogonal grid alignment is required as well (as discussed in Caveat (4) above) then discrete shock detection and tracking[25] should be considered. Ultimately, the algorithmic complexity and overhead of adapting suitable grids around shocks may be no less onerous than that required to detect and track discrete shocks as they move across the background grid and modify the reconstruction algorithm when a discrete shock cuts an edge.

Code Validation

Validation of computational aerothermodynamics codes requires access to both ground- and flight-data. In some cases, Direct Numerical Simulation (DNS) of simple, "unit" problems is recommended to calibrate physical models.

Flight data: Comparison to flight data is the most important source of validation for the suite of physical models required for aerothermodynamic simulation. Flight data[1,2] (STS – accelerations and heating rates, FIRE 2 – convective and radiative heating, Mars Pathfinder – accelerations, RAM-C – electron number densities) are important, particularly for new vehicles that are modest perturbations of tested configurations. However, boundary conditions are not always well defined in flight and integrated, multi-physics effects usually compromise validation of component physical models. For example, in the FIRE 2 data set there are multi-temperature, chemical kinetics models; thermal relaxation models; and surface catalytic boundary conditions (among others) that must all be right to agree with measured data. Offsetting errors may not be identified – one may only conclude that a specific set of models is consistent with the measured data set.

Facility data: Ground-based tests provide the best opportunity to measure boundary conditions and probe the flowfield with sufficient detail to validate physical models. The facilities are not perfectly quiet and often the flows are neither perfectly uniform nor perfectly steady. As enthalpies are increased flow quality and test times become more problematic. New facilities may alleviate some of these difficulties[26]. However, the problematic conditions are accessible to measurement and subsequent specification in the simulation. One strives for benchmark tests that are simple to simulate (axisymmetric, steady, uniform, laminar - if turbulence is not specifically being studied) but in reality the validation process must accommodate the complexities of the test. Consider the following validation tests as an example of this process.

A series of experiments to measure pressure and heating for code validation involving hypersonic, laminar, separated flows was conducted at the Calspan-University at Buffalo Research Center (CUBRC) in the Large Energy National Shock (LENS) tunnel. These tests were the focus of a "workshop" for hypersonic applications organized by Holden and Harvey[27] that should be used as a model for ongoing code validation work. (Its format evolved from earlier, groundbreaking workshops with broader focus on a variety of high-speed simulations[28].) The experimental data were not available to the authors until the conclusion of the workshop session, held at the AIAA Aerospace Sciences Meeting in Reno (2001). Participants transferred their results in prescribed formats to the organizers for public display in the final presentation of the session with respect to experimental data and others' simulations. One set of experiments involve Mach 9.5 and Mach 11.3 N_2 flow over a hollow cylinder-flare with 30^o flare angle at several Reynolds numbers sustaining laminar, separated flow. Truncated and extended flare configurations were considered. A second set of experiments, at similar conditions, involved flow over a sharp double cone (Fig. 12) with fore-cone angle of 25^o and aft-cone angle of 55^o. Both sets of experiments included 30^o compressions.

Location of separation is extremely sensitive to the level of grid refinement in the numerical predictions. For example, at conditions for simulation of Run 28 for the sharp, double cone (V_∞ = 2664. m/s, ρ_∞ = 0.000655 kg/m^3, T_∞ = 185.6 K, M_∞ = 9.59, and Re_∞ = 144010. m^{-1}), a grid converged solution for onset of separation is not achieved until a grid density equal to 512 streamwise by 256 normal. (A plot of this grid in half column format would show almost no white space between grid lines.) A simulation using half the number of nodes in both coordinate directions yields a 20% smaller separation

zone. The reflected wave pattern at reattachment (Fig. 13) is very complex. The value of an adjoint based grid adaptation capability (recall Fig. 4 relative to Fig. 3) for a problem like this cannot be overstated. The current grid is highly refined even in areas of smooth flow and without adaptation, including automatic coarsening, the requirements for this same problem at angle of attack (3D flow) is estimated to be of order of 10^6 nodes.

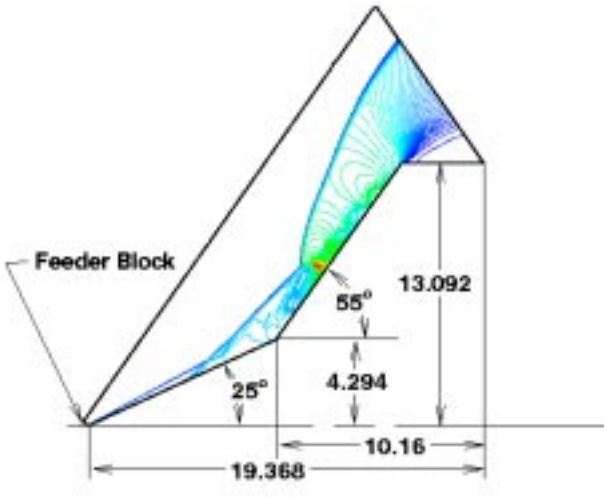

Fig. 12: Sharp, double cone (SDC) and computational domain bounding pressure contour solution.

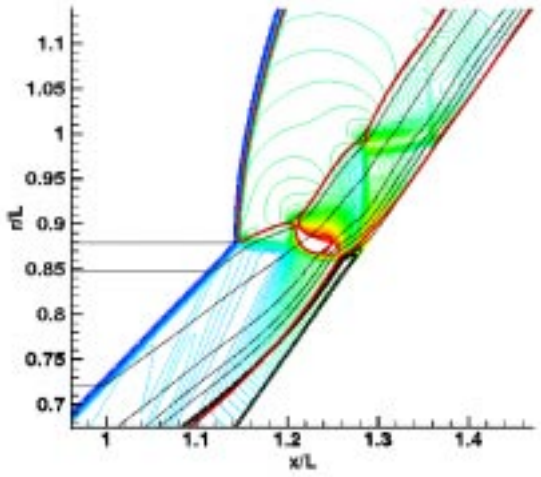

Fig. 13: Detail of interaction region for Run 28 with pressure contours (thin, multi-colored lines), streamlines (thin, black lines), and sonic line (thick, red line).

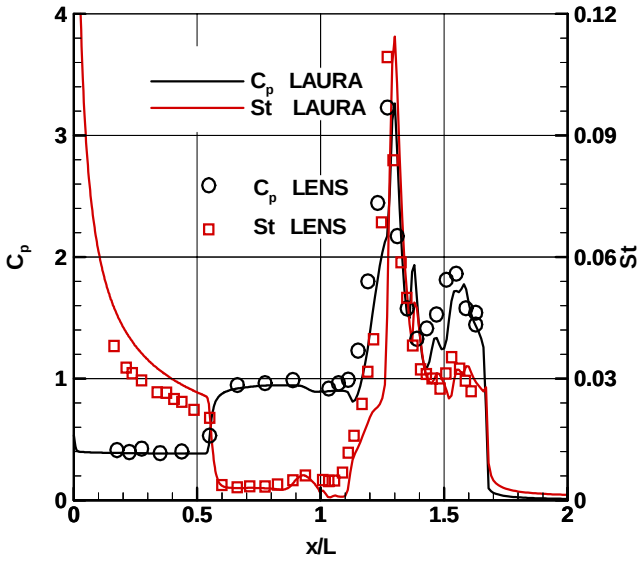

Fig. 14: Surface pressure and heating distributions for Run 28.

The most interesting development from this study concerned the simulation of heat transfer and pressure along the forward portion of the sharp cone. This region in front of the separation region was expected to be the easiest to "get right" and yet was consistently overpredicted by the participants (Fig. 14). A follow-on computational study by Candler et al.[29] showed that thermal nonequilibrium effects in the expansion from the shock tube nozzle and turbulent transition on the tunnel walls were required in the simulation to recover proper freestream conditions. When these effects were included in the simulation with a model for vibrational energy accommodation at the surface, the measured forebody heating and pressures were recovered. These phenomena had less severe impact on the flow in the interaction region where simulations had been in relatively good agreement with experimental data – the thermal effects had sufficient time to equilibrate in the recirculating flow.

These follow-on efforts by Candler et al.[29] and in a related NATO Research and Technology Organization (RTO) study[30] underscore the proposition that future code validation tests will require more complete simulation of the facility flow in addition to simulation around models. Consider for example recent comparisons with high enthalpy tests in T5[31] and X2[32]. The quality of the comparisons is encouraging but uncertainty exists in the specification of boundary conditions. Benchmark simulations of facility flow (time accurate, three-dimensional, appropriate thermochemical models) over a range of operating conditions and atmospheres

will need to be part and parcel of future validation studies. As in the case of flight data, there are multi-physics effects that obscure the validation; however, a richer opportunity to make measurements can be exploited to better quantify uncertainties.

DNS: On top of any list for code validation needs is prediction of hypersonic transition and turbulent heating levels. This is especially true for vehicles that are designed to cruise at hypersonic conditions (NASP, X-43) as opposed to enduring a hypersonic environment during ascent and entry (STS). Understanding the effects of turbulence on mixing and ignition delay are critical priorities for the scramjet community. The goal here is to calibrate the sub-grid scale physics in an LES or multi-equation turbulence models using DNS and then validate the new model with experiment. In theory, DNS can gather statistics on a fine scale inaccessible to experimental methods. Dong and Zhong in this regard discuss recent efforts[33] for structured grid, high-order (5^{th}), shock fitted algorithm to simulate hypersonic, blunt body flow. It is interesting to note that the problems associated with high-order shock capturing are avoided in their shock fitted approach.

Software Engineering

As computational aerothermodynamic simulation codes grow in complexity, issues of software engineering (how one develops, integrates, and maintains software) become critically important. The HEFSS team has struggled with software engineering issues that pit code modularity and maintainability versus code efficiency. At one extreme, future research and development users of the software need to be able to modify algorithms, add functionality, couple new physics, and expand boundary condition options with confidence that the task will not take weeks to figure out and their changes will not break something else. At the other extreme, application users of the code would like for it to run as quickly as possible so that high fidelity information can be brought more effectively into the design process. Our team is far from unique in facing these issues. We have adopted some strategies that work well for us given our initial conditions (diverse expertise in three codes) and environment (government lab).

The HEFSS team includes a dozen people across four branches at Langley who actively create and modify code on an ongoing basis. It is adopting Extreme Programming (XP) methods in this endeavor within a research environment[3435]. This approach has been a major culture shift – but it is one we believe essential in order to engage the many elements of this project. For example, the merging of mixed-elements, adjoint-based optimization algorithms, implicit line solves, and hypersonic physical models progressed simultaneously on a continuously upgraded suite of modules. Two elements of XP that have been critical in achieving our goals are continuous testing/builds and pair programming.

Testing: Source code is maintained in a Concurrent Version System (CVS – http://www.cvshome.org) repository, (one of several revision control systems available for software management). Every "expert" on the team is responsible for defining a sufficient number of tests to cover software functionality within their domain. The tests (over 250 and counting) run on a continuous basis and check compilation and execution for a variety of applications on several platforms using a fresh checkout of code from the repository. All team members are encouraged to "commit" their work to the repository as it develops as quickly as possible without any requirement to obtain approval from a software manager. (A CVS "commit" revises software in the repository accessed by all users.) In this environment, one finds that if too much time passes between "commits" of new material then the resolution of software conflicts becomes more tedious and difficult. If "commits" are too careless, without adequate checks using the test suite, the continuous builds and tests will catch a failure and automatically notify the entire team. In this regard, peer pressure works to encourage good programming practice.

Pair Programming: Pair programming is an effective way of growing knowledge about code. Team members work in pairs to develop code and implement algorithms in real time. More people have detailed knowledge of code and programming strategies because of these pair programming sessions. The non-expert participant (for a particular algorithm or physical model) generally is better suited to define the level of comments required to instruct future developers.

Implementation: Our implementation of XP arose from a series of seminars organized by two advocates of XP within our team. We have developed a strategy that works for us and continues to evolve. In my opinion, the process would never have been effectively implemented had it been mandated from above – a healthy group dynamic is critical to its success.

Concluding Remarks

Opportunities to advance the state-of-art in algorithms, grid generation and adaptation, and code validation are identified with emphasis on the needs

of computational aerothermodynamics. Unstructured grid algorithms with adjoint based adaptation capabilities provide the greatest opportunity for next generation hypersonic flow simulation and vehicle design. The primary justifications for investment in such technology arise from the efficiency in generating an initial, workable grid from CAD files (as compared to multiblock structured, C0 continuous or overset grids) and in the ability to adapt these grids using adjoint algorithms. Adjoint adaptation provides an objective metric of grid quality based on user specified tolerances on errors associated with grid convergence. It provides logic for coarsening as well as refining grids so that only the grid resources required for attaining the target error norms are used in the simulation. However, unstructured grid algorithms in hypersonic applications exhibit shortcomings in regard to simulation of heating – a fundamental requirement of computational aerothermodynamics. These problems stem from difficulties in providing high-order accurate representation of gradients using high aspect ratio tets (usually overcome with use of prisms in the near wall region), entropy gradients associated with jagged shock captures flowing into the boundary layer, and the adverse effects of limiters in an unstructured system.

Examples of algorithmic effects on stagnation region heating are provided herein. Tests are conducted on hypersonic flow over cylinders using a highly biased, unstructured grid discretization. The stagnation region heating is especially sensitive to details of the inviscid flux definition. A Symmetric Total Variation Diminishing (STVD) algorithm provides the best results of options tested in this environment (biased tets all the way to the wall); however, solution quality (as judged by spanwise constancy) is marginally acceptable for this case. Further improvement using multi-dimensional, upwind algorithms and more flexible, mixed-element grid topologies will be sought in future work. Anisotropic, mixed-element grid adaptation that better aligns with shock and high gradient regions may relax the need for additional algorithmic improvement in these hypersonic applications.

Validation of new and existing algorithms continues to be a critical requirement of computational aerothermodynamics. Code validation based on experimental data of "unit" flow problems is an ideal that enables evaluation of specific simulation capabilities and requirements. As facilities strive to push the gas harder to achieve high enthalpy hypersonic flow, it becomes increasingly difficult to provide well defined boundary and initial conditions for "simple", axisymmetric flow simulation. The CFD validation process must address the need to extend the simulation across the facility itself to define the core flow feeding the "simple" configuration and test. An example of this process by Candler et al.[29] pertaining to validation data from Holden et al.[27] showed that facility simulation was required to better quantify thermal nonequilibrium effects in the free stream and their consequent effect on heating and pressure on the forward portion of a sharp cone.

Finally, the critical (and evolving) role of agile software engineering practice in the development of simulation capability is noted. Introduction of extreme programming (XP) into a research-oriented team was initially met with skepticism but has been welcomed as experience is gained. The primary reason for the change of heart is the recognition of how quickly diverse capabilities by many authors can be merged in a shared suite of modules providing real time access to the latest advances in physical models, boundary conditions, and algorithms.

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References

[1] Gnoffo, P. A.; Weilmuenster, K. J.; Hamilton, H. H. II; Olynick, D. R.; Venkatapathy, E.: "Computational Aerothermodynamic Design Issues for Hypersonic Vehicles," JSR, Vol. 36, No. 1, pp 21-43, Jan. 1999.
[2] Gnoffo, Peter A.: "Planetary-Entry Gas Dynamics," Ann. Rev. Fluid Mech. 1999, 31:459-94.
[3] Thomas, J. L. et al.: "Opportunities for Breakthroughs in Large-Scale Computational Simulation and Design," NASA TM 2002-211747, June 2002.
[4] Cheatwood, F. M. and Gnoffo, P. A.: "User's Manual for the Langley Aerothermodynamic Upwind Relaxation Algorithm (LAURA)", NASA TM 4674, April 1996.
[5] White, J. A.; Morrison, J. H.: "A Pseudo-Temporal Multi-Grid Relaxation Scheme for Solving the Parabolized Navier-Stokes Equations," AIAA Paper 2002-0143, Jan 2001.
[6] Anderson, W. K.; Bonhaus, D. L.: "An Implicit Upwind Algorithm for Computing Turbulent Flows on Unstructured Grids," Computers and Fluids, Vol. 23, No. 1, pp 1-21, 1994.
[7] Jones, W. T.: "An Open Framework for Unstructured Grid Generation," AIAA Paper 2002-3192, June 2002.

[8] Castro Diaz, M. J.; Hecht, F.; Mohammadi, B.: "New Progress in Anisotropic Grid Adaptation for Inviscid and Viscous Flows Simulations," INRIA No. 2671, Oct. 1995.
[9] Venditti, D. A.: "Grid Adaptation for Functional Outputs of Compressible Flow Simulations" PhD Dissertation at Massachusetts Institute of Technology, Dept. of Aero. and Astro., June 2002.
[10] Venditti, D. A.; Darmofal, D. L.: "Grid Adaptation for Functional Outputs: Application to Two-Dimensional Inviscid Flows," J. Comput. Phys., 176, pp 40-69, 2002.
[11] Anderson, W. K.; Venkatakrishnan, V.: "Aero-dynamic Design Optimization on Unstructured Grids with a Continuous Adjoint Formulation," AIAA 97-0643, Jan. 1997.
[12] Atwood, C.: "Computation of a Controlled Store Separation from a Cavity," AIAA J. Aircraft, Vol. 32, No. 4, July-August 1995, pp. 846-852.
[13] Togashi, F., Nakahashi, K., Ito, Y., Shinbo, Y., Iwamiya, T., "Flow Simulation of NAL Experimental Supersonic Airplane/Booster Separation Using Overset Unstructured Grids", Computers & Fluids, Vol. 30, pp. 673-688, 2001.
[14] Aftomis, M.: "3D Applications of a Cartesian Grid Euler Method," AIAA 95-0853, Jan. 1995. See also: http://people.nas.nasa.gov/~aftosmis/cart3d/cart3Dhome.html
[15] Lesieur, M.; Comte, P.: "Large-Eddy Simulations of Compressible Turbulent Flows," in AGARD Report 819, Turbulence in Compressible Flows, pp 4-1 – 4-39, June 1997.
[16] Lohner, R.: "Generation of Unstructured Grids Suitable for RANS Calculations," AIAA-99-0662, Jan. 1999.
[17] Aftosmis, M.; Gaitonde, D.; Tavares, T. S.: "Behavior of Linear Reconstruction Techniques on Unstructured Meshes," AIAA J., Vol. 33, No. 11, Nov. 1995, pp2038-2049.
[18] Roe, P. L.: "Approximate Riemann Solvers, Parameter Vectors, and Difference Schemes," J. Comput. Phys., vol. 43, no. 2, Oct. 1981, pp. 357-372.
[19] Barth, T. J.: "Numerical Aspects of Computing High-Reynolds Number Flows on Unstructured Meshes," AIAA Paper 91-0721, 1991.
[20] Barth, T. J.; Jespersen, D. C.: "The Design and Application of Upwind Schemes on Unstructured Meshes," AIAA Paper 89-0366, Jan. 1989.
[21] Venkatakrishnan, V.: "Convergence to Steady-State Solutions of the Euler Equations on Unstructured Grids with Limiters," J. Comp. Phys, 118:120-130, 1995.
[22] Yee, H. C.: "Construction of Explicit and Implicit Symmetric TVD Schemes and Their Applications," J. Comput. Phys., vol. 68, no. 1, Jan. 1987, pp. 151-179
[23] Van der Weide, E. "Compressible Flow Simulation On Unstructured Grids Using Multi-Dimensional Upwind Schemes," Ph.D thesis, Aero. Eng., Delft University of Technology, 1998.
[24] Houtman, E.M.; Van der Weide E.; Deconinck, H. and Bakker, P.O.: "Computational Analysis of Base Flow/Jet Plume Interaction," Proc. 3d European Symp. on Aerothermodynamics for Space Vehicles, ESA SP-426, pp 605-612, 1998.
[25] Moretti, G.:Efficient Euler Solver with Many Applications," AIAA Journal, Vol 26. No. 6 (1988), p655-660.
[26] Mansfield, D. K.; Grinstead, P. J.; Howard, P. J.; Brown, G. L.; Girgis, I.; Miles, R. B.; Lipinski, R.; Pena, G.; Schneider, L.; Howard, R.: "A 1 MW Radiatively-Driven Hypersonic Wind Tunnel Experiment," AIAA 2002-3130, June 2002.
[27] Holden, M. and Harvey, J.: "Comparisons Between Experimental Measurements over Cone/Cone and Cylinder /Flare Configurations and Predictions Employing DSMC and Navier-Stokes Solvers," AIAA 2001-1031, January 2001.
[28] Borrelli, S.; Grasso, F.; Marini, M.; Periaux, J. (eds.): First Europe-US High Speed Flow Field Database Workshop, Published by AIAA, ISBN 1-56347-341-0, 1997.
[29] Candler, G. V.; Nompelis, I.; Druguet, M.-C.; Holden, M. S.; Wadhams, T. P.; Boyd, I. D.; Wang, W-L.: "CFD validation for hypersonic flight - Hypersonic double-cone flow simulations," AIAA Paper 2002-0581, Jan. 2002.
[30] Candler, G. V.; Nompelis, I.; "CFD Validation for Hypersonic Flight - Real GasFflows," AIAA Paper 2002-0434, Jan. 2002.
[31] Rasheed, A.; Fujii, K.; Hornung, H. G.; Hall, J. L.: "Experimental investigation of the flow over a toroidal aerocapture ballute," AIAA Paper 2001-2460, June 2001
[32] Mclntyre, T. J.; Bishop, A. I.; Rubinsztein-Dunlop, H.; Gnoffo, P. A.: "Experimental and Numerical Studies of Ionizing Flow in a Super-Orbital Expansion Tube," AIAA 2001-0752, Jan. 2001
[33] Dong, H. and Zhong, X.: "Time-accurate Simulations of Hypersonic Boundary Layer Stability and Transition over Blunt Bodies Using Implicit Parallel Algorithms," AIAA Paper 2002-0156, Jan. 2002.
[34] Kleb, W. L., Nielsen, E. J., Gnoffo, P. A., Park, M. A.: "Team Software Development in Support of Fast Adaptive AeroSpace Tools (FAAST)," AIAA-2003-3978, June 2003.
[35] Wood, W. A.; Kleb, W. L.: "Exploring XP for Scientific Research," IEEE Software, Vol. 20, No. 3, pp. 30-36, May/June 2003.